

REPORT

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**Rigorous analysis for
estimating the orientation of
cubic crystals**

**L N McCartney
K Clay**

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Rigorous analysis for estimating the orientation of cubic crystals

L N McCartney
Industry and Innovation Division

Kath Clay
Hexmat Materials Consultancy Ltd

ABSTRACT

This report describes a rigorous mathematical method of defining angles that may be used to characterise the orientation of cubic crystals with respect to a given set of reference axes. Extensive use is made of unit vectors and their transformation by successive rotations about the three principal axes of the crystal.

The report adheres to a notation and definitions that are used in the European Gas Turbine Industry, even though the approach is not optimal from a mathematical viewpoint.

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National Physical Laboratory
Hampton Road, Teddington, Middlesex, TW11 0LW

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Approved on behalf of the Managing Director, NPL,
by Dr M G Cain, Knowledge Leader, Materials Team
authorised by Director, Industry and Innovation Division

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1. INTRODUCTION

The objective of this report is to define clearly one method of determining the orientation of a cubic crystal relative to a reference set of axes. Crystal orientation can be defined by three angles of rotation that are applied during three successive transformations about axes that are related to a set of reference coordinates and their associated orthogonal axes, which are associated with the structure of a cubic crystal. The method adopted attempts to adhere to that which is used by the European Gas Turbine Industry when interpreting measurements obtained from an X-ray diffraction method of determining the orientation of cubic crystals.

The key task is the interpretation of the spots on images obtained when determining crystal orientation using the Back Reflection Laue (BRL) method (see [1]). The BRL patterns are captured on wet-film and images analysed when looking from behind the film towards the crystal that generated the spots. Alternatively, use is sometimes made of Polaroid film so that images have to be analysed when observed in the opposite direction (i.e. looking from the crystal towards the film). More recent developments with CCD detectors have enabled live images to be captured and analysed without recourse to the use of film. In this report it is assumed that BRL images have been obtained using the wet-film method, which have been analysed in the traditional way.

An important issue is the unambiguous definition of the orientation angles that are used to describe crystal orientation relative to a set of orthogonal reference axes whose location and directions are determined by the experimental situation. Rectangular Cartesian coordinates will be used in this report and a choice has to be made regarding whether the axes are left- or right-handed. **The European Gas Turbine Industry usually makes use of left-handed sets of axes, and this convention will be adopted everywhere in this report.** Also, all angles will be defined in radians so that they are dimensionless and can be used directly in trigonometrical formulae. When angles are described in degrees, this does not imply a change of dimension, only a change of measurement scale.

2. BACK REFLECTION LAUE METHOD

It is now useful to describe in detail (based on reference [1]) the nature of BRL methodology that leads to a pattern of spots on a planar rectangular film that can then be interpreted to determine the orientation of a crystal relative to a set of reference axes. The reference axes are chosen to be parallel to the incident X-ray beam and the edges of the film such that the beam passes through the origin. When a very slender beam of X-rays impinges on a set of parallel atomic planes in a cubic crystal, the beam undergoes diffraction driven back-reflection. This leads to multiple beams satisfying Bragg diffraction conditions, which arise from multiple planes of reflection whose orientations are determined by the various reflecting planes that can be identified in the crystal. These reflected beams intersect a planar film, which is normal to the incident beam, and create a pattern of BRL spots that can be used to determine the orientation of the crystal relative to the set of reference axes defined by the direction of the beam and the orientation of the film about the axis associated with the incident beam, which must pass through a hole in the film.

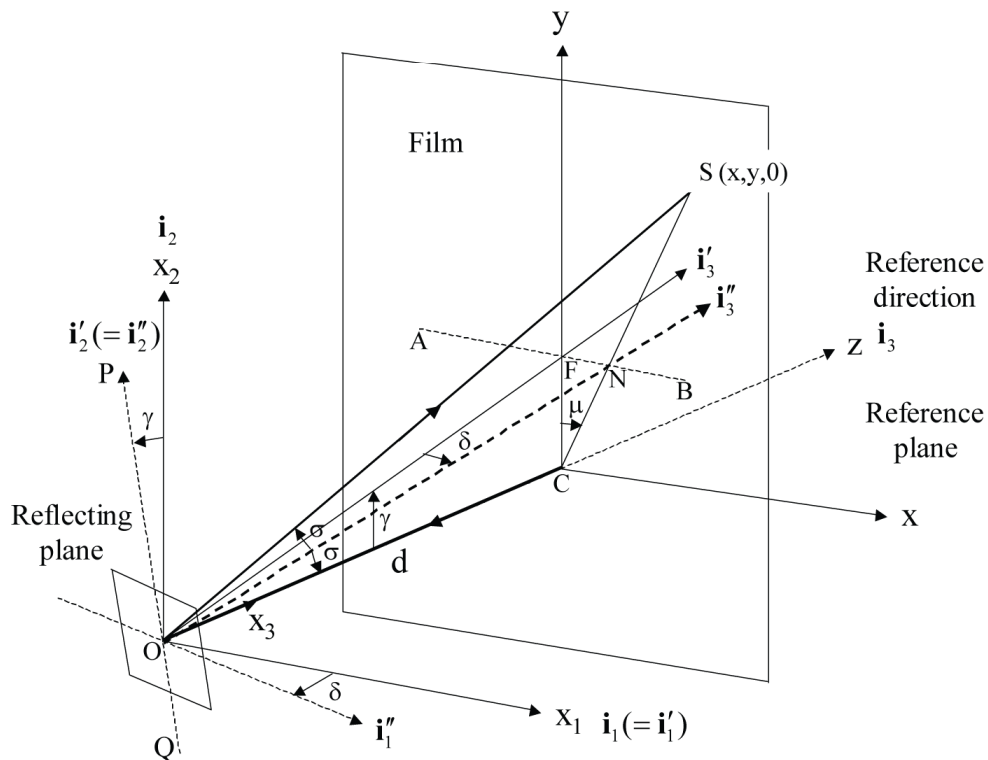


Figure 1: Diagram illustrating Back Reflection Laue technique.

A left-handed set of rectangular Cartesian reference coordinates (x, y, z) are now introduced, as shown in Fig.1, such that the x and y axes are in the plane of the film and parallel to the edges of the film. The X-ray beam is located on the z -axis and is directed from the origin C towards negative values of z . The incident X-ray beam CO is reflected at point O on a reflecting plane in the crystal as illustrated in Fig.1 that is a distance d from the point C . On reflection the beam is directed towards the film plate and intersects the plane of the film at the point S having coordinates $(x, y, 0)$. The normal to the reflecting plane passing through the point O of this plane intersects the film at the point N . The normal ON and both the incident ray CO and reflected ray OS are co-planar. The normal ON is parallel to the $(0,0,1)$ direction of the crystal after consecutive rotations by the angles γ and δ . The straight line AB , which is parallel to the x -axis, passes through N and intersects the y -axis at the point F . An axis PQ on the reflecting plane can be identified such that, when the reflecting plane is rotated about this axis, the intersection of the normal ON with the film will move along the straight line AB . The line AB must be a straight line because it is the intersection of the planar film with the plane that is generated when the normal ON is rotated about the axis PQ . The location of the point N on the film may be described by the angles γ and δ as shown in Fig.1, where their positive direction is indicated by arrows. The angle of incidence of the X-ray beam is denoted by σ which is also the angle of reflection. The angle FCN is denoted by μ . It is easily shown that [1]

$$\tan \mu = \frac{\tan \delta}{\sin \gamma}, \quad \tan \sigma = \frac{\tan \delta}{\sin \mu \cos \gamma}, \quad x = d \sin \mu \tan 2\sigma, \quad y = d \cos \mu \tan 2\sigma.$$

It follows from the discussion of BRL patterns in reference [1] that the loci of the point S shown in Fig.1, as either γ or δ is varied keeping the other angle fixed, generates curves in the xy-plane that are symmetric about both the x- and y-axes. It is useful to investigate the nature of the curves generated, which would rotate about the z-axis without changing shape when the crystal is rotated about the normal ON to the reflection plane.

It can be shown that, when the angle γ is held fixed while the angle δ varies, the values of x and y generating one family of curves are related by

$$y = b \pm b \sqrt{\frac{x^2}{a^2} + 1}, \quad \text{where } a = \frac{1}{\sqrt{1 - \tan^2 \gamma}}, \quad b = \frac{\tan \gamma}{1 - \tan^2 \gamma}.$$

The curves generated in the xy-plane are hyperbolae of the form

$$\left(\frac{y-b}{b}\right)^2 + \frac{x^2}{a^2} = 1.$$

When the angle δ is held fixed while the angle γ varies, the values of x and y generating the other family of curves are related by

$$x = \pm \frac{\tan \delta}{1 - \tan^2 \delta} \sqrt{2 \left[1 + (1 - \tan^2 \delta) y^2 \pm \sqrt{1 + (1 - \tan^4 \delta) y^2} \right]}.$$

Real values of x can only be obtained from the following expression

$$x = \pm \frac{\tan \delta}{1 - \tan^2 \delta} \sqrt{2 \left[1 + (1 - \tan^2 \delta) y^2 + \sqrt{1 + (1 - \tan^4 \delta) y^2} \right]}.$$

The curves generated by this formula in the xy-plane are *not* hyperbolae, as suggested in reference [1].

A new set of reference axes is now introduced (x_1, x_2, x_3) having origin at the reflection point O within the crystal so that $x_1 = x$, $x_2 = y$, $x_3 = d + z$.

The new set of left-handed reference axes are obtained by translating the axes (x, y, z) a distance d along the negative part of the z-axis to the point O, as shown in Fig.1. The new reference axes can then be transformed to align with the principal directions of a cubic crystal simply by rotating about three axes in turn as will now be described.

The orientation angles of interest belong to two different categories. The first category comprises three measured angles (γ, δ, α) where γ and δ have been described above, and where α is a third measured angle to be described below. The second category is a set of derived angles that are determined from the measured angles as described in Table 1 (taken from the NPL Good Practice Guide [2]).

Table 1: Derived angles from directly measured angles (European Convention).

Derived angle	Formula	Equation no. in this report
$\kappa_{\text{true}} (\kappa_{\text{true}})$	$\tan \kappa_{\text{true}} = \tan \alpha \cos \gamma / (\cos \delta - \tan \alpha \sin \gamma \sin \delta)$	(28)
$\omega (\omega)$	$\tan \hat{\omega} = \sin \gamma / \tan \delta$	(29) and Table 2
$\theta (\theta)$	$\cos \theta = \cos \gamma \cos \delta$	(36)
$\kappa (\kappa)$	$\kappa = \kappa_{\text{true}} - \arctan (\tan \gamma \sin \delta)$	(41)
$\rho (\rho)$	$\rho = \arctan (\tan \gamma / \sin \delta) - \kappa_{\text{true}}$	(45), (46) and Tables 3, 4

3. SUCCESSIVE TRANSFORMATION OF AXES

The *left-handed* set of rectangular Cartesian reference coordinates (x_1, x_2, x_3) , with unit vectors $\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3$ directed towards positive values of the coordinates, is used to define the principal directions of a cubic crystal, as shown in Fig. 2. This set of axes, centred on the reflecting plane in the crystal, are known as the reference axes. The x_3 -direction (i.e. the direction of the unit vector $\mathbf{i}_3$) is known as the reference direction that can be associated with, for example, a solidification direction when manufacturing single crystals or a geometrical feature. Three successive rotations will now be applied about the x_1 axis, and the transformed x_2 and x_3 axes.

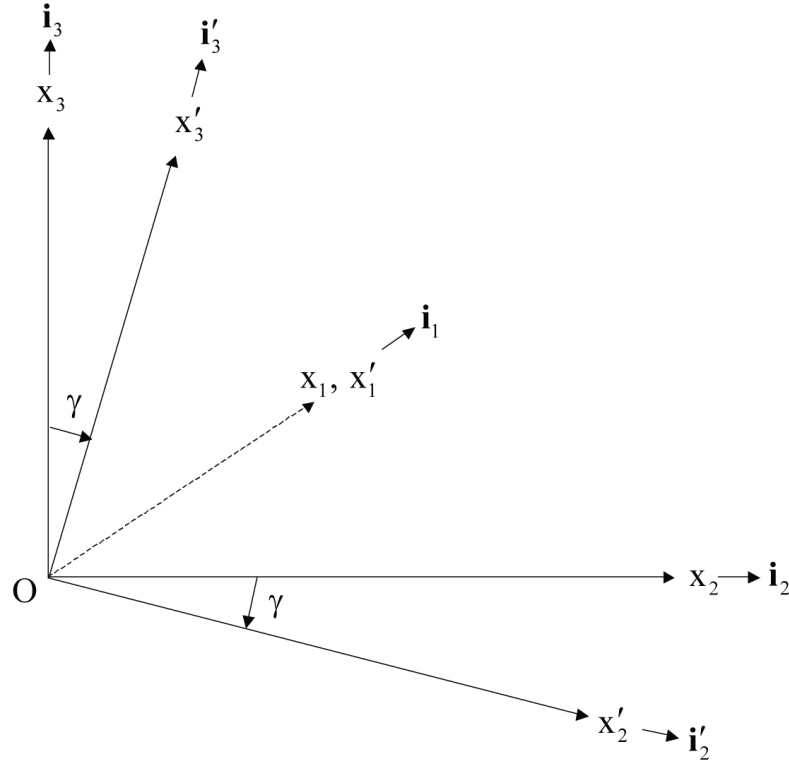


Figure 2: Diagram of the reference coordinates (x_1, x_2, x_3) together with a first rotation of the reference axes by an angle γ about the x_1 axis.

The first rotation is the rotation of the reference axes by an angle γ about the x_1 axis, which is positive when described in a *clockwise* direction when looking from the origin to positive values of $x_1 (= x'_1)$, as illustrated in Fig. 2. The reference axes then transform to a new set of axes (x'_1, x'_2, x'_3) with unit vectors $\mathbf{i}'_1, \mathbf{i}'_2, \mathbf{i}'_3$ directed towards positive values of the transformed coordinates, as shown in Fig. 2. The direction of measuring positive values of the angle γ corresponds to the directions shown by arrows in Figs. 1 and 2. Any point in space can be represented by the vector $\mathbf{x}$ (a first order tensor) as follows

$$\mathbf{x} = x_1 \mathbf{i}_1 + x_2 \mathbf{i}_2 + x_3 \mathbf{i}_3 = x'_1 \mathbf{i}'_1 + x'_2 \mathbf{i}'_2 + x'_3 \mathbf{i}'_3. \quad (1)$$

The unit vectors are related as follows (see Appendix 1 for an example derivation)

$$\begin{aligned} \mathbf{i}_1 &= \mathbf{i}'_1, & \mathbf{i}'_1 &= \mathbf{i}_1, \\ \mathbf{i}_2 &= \cos \gamma \mathbf{i}'_2 + \sin \gamma \mathbf{i}'_3, & \mathbf{i}'_2 &= \cos \gamma \mathbf{i}_2 - \sin \gamma \mathbf{i}_3, \\ \mathbf{i}_3 &= -\sin \gamma \mathbf{i}'_2 + \cos \gamma \mathbf{i}'_3, & \mathbf{i}'_3 &= \sin \gamma \mathbf{i}_2 + \cos \gamma \mathbf{i}_3. \end{aligned} \quad (2)$$

On using (1) and (2), the transformation of a set of Cartesian coordinates (x_1, x_2, x_3) to (x'_1, x'_2, x'_3) by a rotation of the x_2 and x_3 axes about the x_1 -axis through an angle γ (as shown in Fig. 2) leads to

$$\begin{aligned} x_1 &= x'_1, & x'_1 &= x_1, \\ x_2 &= x'_2 \cos \gamma + x'_3 \sin \gamma, & x'_2 &= x_2 \cos \gamma - x_3 \sin \gamma, \\ x_3 &= -x'_2 \sin \gamma + x'_3 \cos \gamma, & x'_3 &= x_2 \sin \gamma + x_3 \cos \gamma. \end{aligned} \quad (3)$$

These relationships can also be established from the geometry shown in Fig. 2 on using suitable constructions. The relations (3) are often written in the following matrix form

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \gamma & \sin \gamma \\ 0 & -\sin \gamma & \cos \gamma \end{pmatrix} \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix}, \quad \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \gamma & -\sin \gamma \\ 0 & \sin \gamma & \cos \gamma \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \quad (4)$$

The second rotation is a rotation of the transformed axes by an angle δ about the x'_2 axis, which is positive when described in an *anticlockwise* direction when looking from the origin towards positive values of $x'_2 = x''_2$, as shown in Fig. 3. The reference axes then transform to a new set of axes (x''_1, x''_2, x''_3) with unit vectors $\mathbf{i}''_1, \mathbf{i}''_2, \mathbf{i}''_3$ directed towards positive values of the coordinates, as shown in Fig. 3. Any point $\mathbf{x}$ in space can then be represented by

$$\mathbf{x} = x_1 \mathbf{i}_1 + x_2 \mathbf{i}_2 + x_3 \mathbf{i}_3 = x'_1 \mathbf{i}'_1 + x'_2 \mathbf{i}'_2 + x'_3 \mathbf{i}'_3 = x''_1 \mathbf{i}''_1 + x''_2 \mathbf{i}''_2 + x''_3 \mathbf{i}''_3. \quad (5)$$

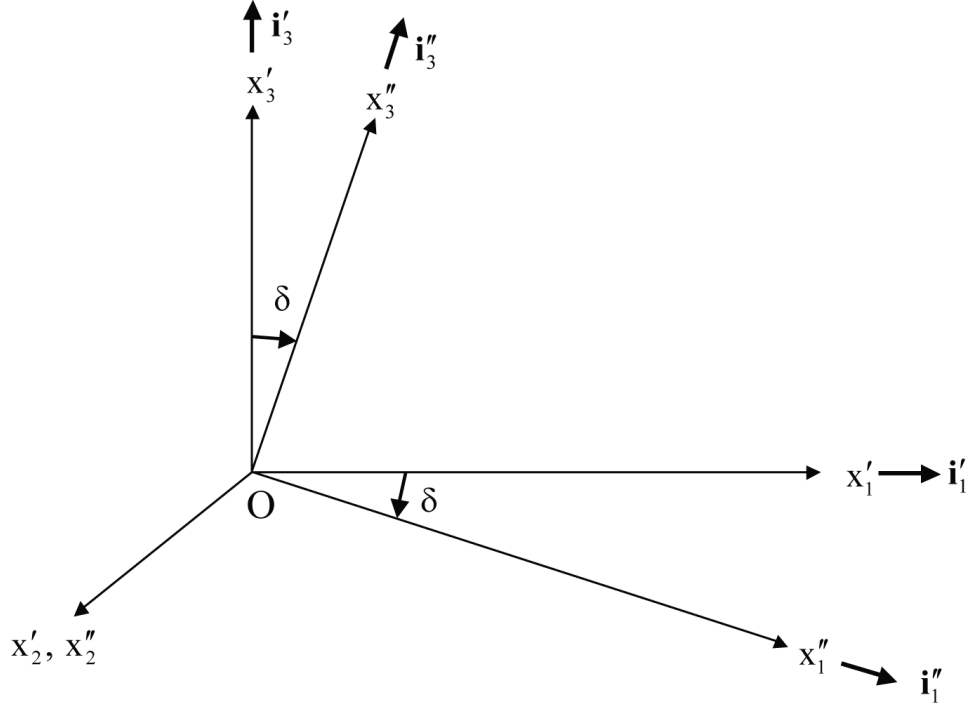


Figure 3: Rotation of the transformed axes by an angle δ about the $x_2' (= x_2'')$ axis.

It then follows that

$$\begin{aligned}
 \mathbf{i}_1' &= \cos \delta \mathbf{i}_1'' + \sin \delta \mathbf{i}_3'', & \mathbf{i}_1'' &= \cos \delta \mathbf{i}_1' - \sin \delta \mathbf{i}_3', \\
 \mathbf{i}_2' &= \mathbf{i}_2'', & \mathbf{i}_2'' &= \mathbf{i}_2', \\
 \mathbf{i}_3' &= -\sin \delta \mathbf{i}_1'' + \cos \delta \mathbf{i}_3'', & \mathbf{i}_3'' &= \sin \delta \mathbf{i}_1' + \cos \delta \mathbf{i}_3'.
 \end{aligned} \tag{6}$$

On using (5) and (6), the transformation of a set of Cartesian coordinates (x_1', x_2', x_3') to (x_1'', x_2'', x_3'') by a rotation of the x_1' and x_3' axes about the x_2' -axis through an angle δ (as shown in Fig. 3) leads to

$$\begin{aligned}
 x_1' &= x_1'' \cos \delta + x_3'' \sin \delta, & x_1'' &= x_1' \cos \delta - x_3' \sin \delta, \\
 x_2' &= x_2'', & x_2'' &= x_2', \\
 x_3' &= -x_1'' \sin \delta + x_3'' \cos \delta, & x_3'' &= x_1' \sin \delta + x_3' \cos \delta.
 \end{aligned} \tag{7}$$

These relationships can also be established from the geometry shown in Fig. 3 on using suitable constructions. The relations (7) are often written in the following matrix form

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} \cos \delta & 0 & \sin \delta \\ 0 & 1 & 0 \\ -\sin \delta & 0 & \cos \delta \end{pmatrix} \begin{pmatrix} x_1'' \\ x_2'' \\ x_3'' \end{pmatrix}, \quad \begin{pmatrix} x_1'' \\ x_2'' \\ x_3'' \end{pmatrix} = \begin{pmatrix} \cos \delta & 0 & -\sin \delta \\ 0 & 1 & 0 \\ \sin \delta & 0 & \cos \delta \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}. \tag{8}$$

It can then be shown using (2) and (6) that

$$\begin{aligned}
\mathbf{i}_1'' &= \cos \delta \mathbf{i}_1 - \sin \delta (\sin \gamma \mathbf{i}_2 + \cos \gamma \mathbf{i}_3), \\
\mathbf{i}_2'' &= \cos \gamma \mathbf{i}_2 - \sin \gamma \mathbf{i}_3, \\
\mathbf{i}_3'' &= \sin \delta \mathbf{i}_1 + \cos \delta (\sin \gamma \mathbf{i}_2 + \cos \gamma \mathbf{i}_3),
\end{aligned} \tag{9}$$

$$\begin{aligned}
\mathbf{i}_1 &= \cos \delta \mathbf{i}_1'' + \sin \delta \mathbf{i}_3'', \\
\mathbf{i}_2 &= \cos \gamma \mathbf{i}_2'' - \sin \gamma (\sin \delta \mathbf{i}_1'' - \cos \delta \mathbf{i}_3''), \\
\mathbf{i}_3 &= -\sin \gamma \mathbf{i}_2'' - \cos \gamma (\sin \delta \mathbf{i}_1'' - \cos \delta \mathbf{i}_3''),
\end{aligned} \tag{10}$$

which are now written in the form

$$\begin{aligned}
\mathbf{i}_1'' &= \cos \delta \mathbf{i}_1 - \sin \gamma \sin \delta \mathbf{i}_2 - \cos \gamma \sin \delta \mathbf{i}_3, \\
\mathbf{i}_2'' &= \cos \gamma \mathbf{i}_2 - \sin \gamma \mathbf{i}_3, \\
\mathbf{i}_3'' &= \sin \delta \mathbf{i}_1 + \sin \gamma \cos \delta \mathbf{i}_2 + \cos \gamma \cos \delta \mathbf{i}_3,
\end{aligned} \tag{11}$$

$$\begin{aligned}
\mathbf{i}_1 &= \cos \delta \mathbf{i}_1'' + \sin \delta \mathbf{i}_3'', \\
\mathbf{i}_2 &= -\sin \gamma \sin \delta \mathbf{i}_1'' + \cos \gamma \mathbf{i}_2'' + \sin \gamma \cos \delta \mathbf{i}_3'', \\
\mathbf{i}_3 &= -\cos \gamma \sin \delta \mathbf{i}_1'' - \sin \gamma \mathbf{i}_2'' + \cos \gamma \cos \delta \mathbf{i}_3''.
\end{aligned} \tag{12}$$

The relations (11) and (12) are now expressed

$$\begin{aligned}
\mathbf{i}_1'' &= \lambda_1 \mathbf{i}_1 + \lambda_2 \mathbf{i}_2 + \lambda_3 \mathbf{i}_3, & \mathbf{i}_1 &= \lambda_1 \mathbf{i}_1'' + \mu_1 \mathbf{i}_2'' + \nu_1 \mathbf{i}_3'', \\
\mathbf{i}_2'' &= \mu_1 \mathbf{i}_1 + \mu_2 \mathbf{i}_2 + \mu_3 \mathbf{i}_3, & \mathbf{i}_2 &= \lambda_2 \mathbf{i}_1'' + \mu_2 \mathbf{i}_2'' + \nu_2 \mathbf{i}_3'', \\
\mathbf{i}_3'' &= \nu_1 \mathbf{i}_1 + \nu_2 \mathbf{i}_2 + \nu_3 \mathbf{i}_3, & \mathbf{i}_3 &= \lambda_3 \mathbf{i}_1'' + \mu_3 \mathbf{i}_2'' + \nu_3 \mathbf{i}_3'',
\end{aligned} \tag{13}$$

where the direction cosines are given by

$$\begin{aligned}
\lambda_1 &= \cos \delta, & \lambda_2 &= -\sin \gamma \sin \delta, & \lambda_3 &= -\cos \gamma \sin \delta, \\
\mu_1 &= 0, & \mu_2 &= \cos \gamma, & \mu_3 &= -\sin \gamma, \\
\nu_1 &= \sin \delta, & \nu_2 &= \sin \gamma \cos \delta, & \nu_3 &= \cos \gamma \cos \delta.
\end{aligned} \tag{14}$$

The next rotation is about the x_3'' -axis by an angle κ , which is positive when described in an *anticlockwise* direction when looking from the origin to positive values of $x_3'' = x_3'''$ as shown in Fig. 4. The reference axes then transform to a new set of axes (x_1''', x_2''', x_3''') with unit vectors $\mathbf{i}_1''', \mathbf{i}_2''', \mathbf{i}_3'''$ directed towards positive values of the coordinates, as shown in Fig. 3.

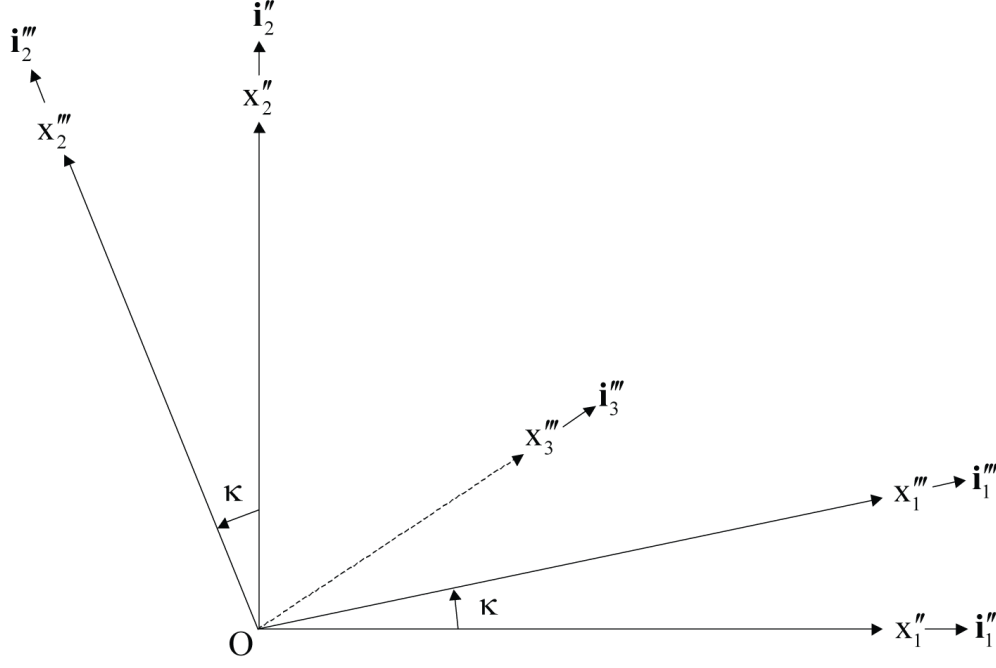


Figure 4: Rotation of the transformed axes by an angle κ about the $x_3'' (= x_3''')$ axis.

Any point $\mathbf{x}$ in space can then be represented by

$$\begin{aligned} \mathbf{x} &= x_1 \mathbf{i}_1 + x_2 \mathbf{i}_2 + x_3 \mathbf{i}_3 = x'_1 \mathbf{i}'_1 + x'_2 \mathbf{i}'_2 + x'_3 \mathbf{i}'_3 \\ &= x''_1 \mathbf{i}''_1 + x''_2 \mathbf{i}''_2 + x''_3 \mathbf{i}''_3 = x'''_1 \mathbf{i}'''_1 + x'''_2 \mathbf{i}'''_2 + x'''_3 \mathbf{i}'''_3. \end{aligned} \quad (15)$$

It then follows that

$$\begin{aligned} \mathbf{i}''_1 &= \cos \kappa \mathbf{i}'''_1 - \sin \kappa \mathbf{i}'''_2, & \mathbf{i}'''_1 &= \cos \kappa \mathbf{i}''_1 + \sin \kappa \mathbf{i}''_2, \\ \mathbf{i}''_2 &= \sin \kappa \mathbf{i}'''_1 + \cos \kappa \mathbf{i}'''_2, & \mathbf{i}'''_2 &= -\sin \kappa \mathbf{i}''_1 + \cos \kappa \mathbf{i}''_2, \\ \mathbf{i}'''_3 &= \mathbf{i}''_3, & \mathbf{i}'''_3 &= \mathbf{i}''_3. \end{aligned} \quad (16)$$

On using (15) and (16), the transformation of a set of Cartesian coordinates (x_1'', x_2'', x_3'') to (x_1''', x_2''', x_3''') by a rotation of the x_1'' and x_2'' axes about the x_3'' -axis through an angle κ (as shown in Fig. 4) leads to

$$\begin{aligned} x_1'' &= x_1''' \cos \kappa - x_2''' \sin \kappa, & x_1''' &= x_1'' \cos \kappa + x_2'' \sin \kappa, \\ x_2'' &= x_1''' \sin \kappa + x_2''' \cos \kappa, & x_2''' &= -x_1'' \sin \kappa + x_2'' \cos \kappa, \\ x_3'' &= x_3''', & x_3''' &= x_3''. \end{aligned} \quad (17)$$

These relationships can also be established from the geometry shown in Fig. 4 on using suitable constructions. The relations (17) are often written in the following matrix form

$$\begin{pmatrix} x_1'' \\ x_2'' \\ x_3'' \end{pmatrix} = \begin{pmatrix} \cos \kappa & -\sin \kappa & 0 \\ \sin \kappa & \cos \kappa & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1''' \\ x_2''' \\ x_3''' \end{pmatrix}, \quad \begin{pmatrix} x_1''' \\ x_2''' \\ x_3''' \end{pmatrix} = \begin{pmatrix} \cos \kappa & \sin \kappa & 0 \\ -\sin \kappa & \cos \kappa & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1'' \\ x_2'' \\ x_3'' \end{pmatrix}. \quad (18)$$

It can then be shown using (11) and (16) that

$$\begin{aligned} \mathbf{i}_1''' &= \cos \delta \cos \kappa \mathbf{i}_1 + (\cos \gamma \sin \kappa - \sin \gamma \sin \delta \cos \kappa) \mathbf{i}_2 \\ &\quad - (\sin \gamma \sin \kappa + \cos \gamma \sin \delta \cos \kappa) \mathbf{i}_3, \\ \mathbf{i}_2''' &= -\cos \delta \sin \kappa \mathbf{i}_1 + (\cos \gamma \cos \kappa + \sin \gamma \sin \delta \sin \kappa) \mathbf{i}_2 \\ &\quad - (\sin \gamma \cos \kappa - \cos \gamma \sin \delta \sin \kappa) \mathbf{i}_3, \\ \mathbf{i}_3''' &= \sin \delta \mathbf{i}_1 + \sin \gamma \cos \delta \mathbf{i}_2 + \cos \gamma \cos \delta \mathbf{i}_3. \end{aligned} \quad (19)$$

These relations lead to the following unit vectors defining the final directions of the original reference axes following the three successive rotations

$$\begin{aligned} \mathbf{i}_1''' &= (\cos \delta \cos \kappa, \cos \gamma \sin \kappa - \sin \gamma \sin \delta \cos \kappa, -\sin \gamma \sin \kappa - \cos \gamma \sin \delta \cos \kappa), \\ \mathbf{i}_2''' &= (-\cos \delta \sin \kappa, \cos \gamma \cos \kappa + \sin \gamma \sin \delta \sin \kappa, -\sin \gamma \cos \kappa + \cos \gamma \sin \delta \sin \kappa), \\ \mathbf{i}_3''' &= (\sin \delta, \sin \gamma \cos \delta, \cos \gamma \cos \delta). \end{aligned} \quad (20)$$

It follows that the directions of the crystal axes, following the three consecutive rotations, are given by the relations

$$\begin{aligned} [1, 0, 0]: & \quad \cos \delta \cos \kappa, \cos \gamma \sin \kappa - \sin \gamma \sin \delta \cos \kappa, -\sin \gamma \sin \kappa - \cos \gamma \sin \delta \cos \kappa, \\ [0, 1, 0]: & \quad -\cos \delta \sin \kappa, \cos \gamma \cos \kappa + \sin \gamma \sin \delta \sin \kappa, -\sin \gamma \cos \kappa + \cos \gamma \sin \delta \sin \kappa, \\ [0, 0, 1]: & \quad \sin \delta, \sin \gamma \cos \delta, \cos \gamma \cos \delta. \end{aligned} \quad (21)$$

The components of these unit vectors correspond exactly with those given in reference [2]. The angles (γ, δ, κ) define the orientation of a cubic crystal with respect to the original set of reference axes.

From (12) and (16) the following relations can be derived, which are the inverse of the relations (20),

$$\begin{aligned} \mathbf{i}_1 &= \cos \delta \cos \kappa \mathbf{i}_1''' - \cos \delta \sin \kappa \mathbf{i}_2''' + \sin \delta \mathbf{i}_3'', \\ \mathbf{i}_2 &= (\cos \gamma \sin \kappa - \sin \gamma \sin \delta \cos \kappa) \mathbf{i}_1''' \\ &\quad + (\cos \gamma \cos \kappa + \sin \gamma \sin \delta \sin \kappa) \mathbf{i}_2''' + \sin \gamma \cos \delta \mathbf{i}_3'', \\ \mathbf{i}_3 &= -(\sin \gamma \sin \kappa + \cos \gamma \sin \delta \cos \kappa) \mathbf{i}_1''' \\ &\quad - (\sin \gamma \cos \kappa - \cos \gamma \sin \delta \sin \kappa) \mathbf{i}_2''' + \cos \gamma \cos \delta \mathbf{i}_3''. \end{aligned} \quad (22)$$

From (15) and (19) it can be shown that

$$\begin{aligned}
 x_1 &= x_1''' \cos \delta \cos \kappa - x_2''' \cos \delta \sin \kappa + x_3''' \sin \delta, \\
 x_2 &= x_1''' (\cos \gamma \sin \kappa - \sin \gamma \sin \delta \cos \kappa) \\
 &\quad + x_2''' (\cos \gamma \cos \kappa + \sin \gamma \sin \delta \sin \kappa) + x_3''' \sin \gamma \cos \delta, \\
 x_3 &= -x_1''' (\sin \gamma \sin \kappa + \cos \gamma \sin \delta \cos \kappa) \\
 &\quad - x_2''' (\sin \gamma \cos \kappa - \cos \gamma \sin \delta \sin \kappa) + x_3''' \cos \gamma \cos \delta,
 \end{aligned} \tag{23}$$

and from (15) and (22) the following inverse relations are obtained

$$\begin{aligned}
 x_1''' &= x_1 \cos \delta \cos \kappa + x_2 (\cos \gamma \sin \kappa - \sin \gamma \sin \delta \cos \kappa) \\
 &\quad - x_3 (\sin \gamma \sin \kappa + \cos \gamma \sin \delta \cos \kappa), \\
 x_2''' &= -x_1 \cos \delta \sin \kappa + x_2 (\cos \gamma \cos \kappa + \sin \gamma \sin \delta \sin \kappa) \\
 &\quad - x_3 (\sin \gamma \cos \kappa - \cos \gamma \sin \delta \sin \kappa), \\
 x_3''' &= x_1 \sin \delta + x_2 \sin \gamma \cos \delta + x_3 \cos \gamma \cos \delta.
 \end{aligned} \tag{24}$$

This completes the development of the mathematical relations that are required to fully understand and characterise the orientation of crystal axes relative to a given set of reference axes.

4. DIRECT MEASUREMENTS FROM LAUE PATTERNS

For the remainder of this report, the symbol κ will be replaced by κ_{true} , as κ is usually used by the European Gas Turbine Industry [2] to represent a different angle that is related to κ_{true} . It is useful to consider first of all the case where the cubic crystal aligns perfectly with respect to the reference axes, a situation that would occur when $\gamma = \delta = \kappa_{\text{true}} = 0$. The crystal is then imagined to be reoriented to its actual position defined by values of the three angles γ , δ , κ_{true} . On referring to Fig.1, it is possible, from the spots forming a BRL pattern that are seen when using the wet-film method, to identify the location N of the point where the line, passing through the point C on the reflecting plane and containing the unit vector $\mathbf{i}_3''$, intersects the film. The location of this point is uniquely identified by the measured angles γ and δ shown in both Fig.1 and Fig. 5. As the third rotation through an angle κ_{true} cannot be measured directly, there is a need to identify a method to estimate this orientation angle from BRL patterns.

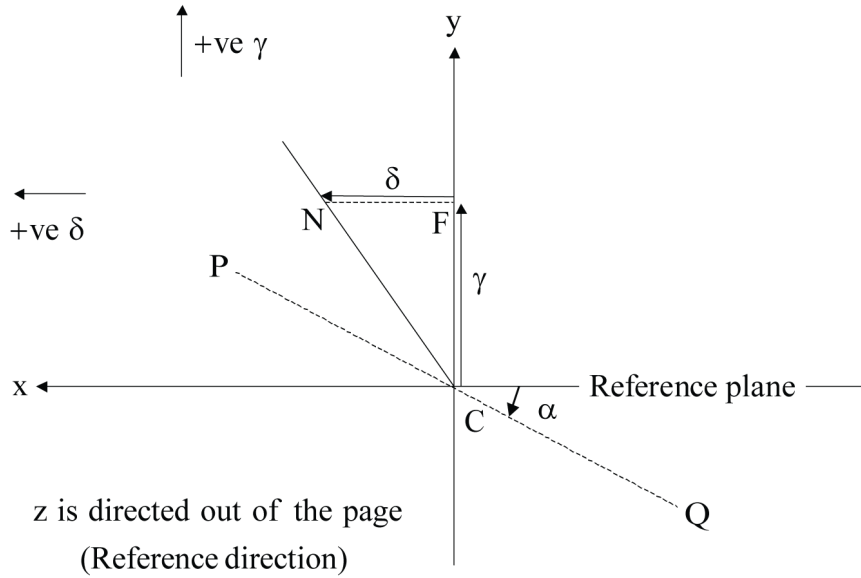


Figure 5: Diagram illustrating angles measured from Laue patterns on wet film (geometry shown assumes $\kappa_{\text{true}} > 0$).

During the imagined rotations of the crystal from the position where $\gamma = \delta = \kappa_{\text{true}} = 0$ to its actual position in the experiment, the intersections of the principal crystal planes with the film will be straight lines that rotate about the point C in the xy-plane of Figs.1 and 5, and about the point O in the x_1x_2 -plane of Fig.6.

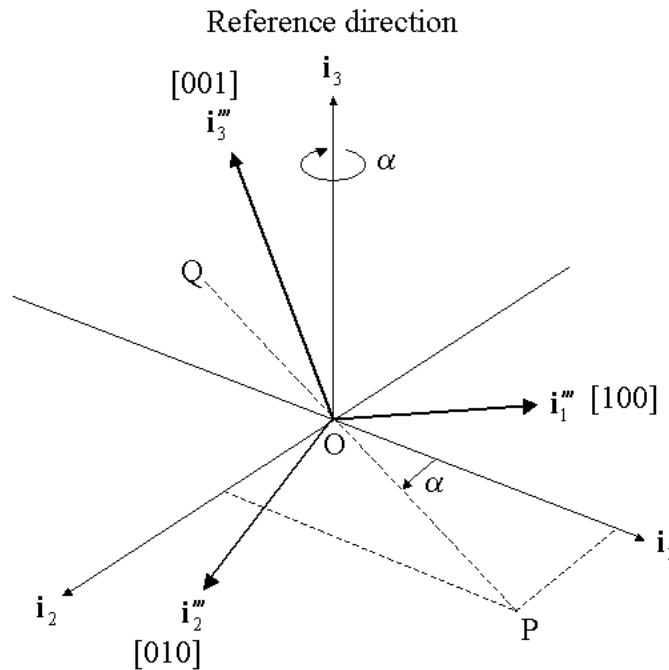


Figure 6: Diagram illustrating the angle α measured from Laue patterns on wet film.

First of all it is useful to focus on the crystal plane that initially coincides with the xz-plane of Fig.1, i.e. the reference plane. The unit vector $\mathbf{i}_2$ is normal to the xz-plane and thus parallel to the y-axis. Following the three successive rotations about three different axes, the unit vector $\mathbf{i}_2$ transforms to the unit vector $\mathbf{i}_2'''$, as shown in Fig. 6.

From (24) the plane $x_2''' = 0$ normal to the unit vector $\mathbf{i}_2'''$ is thus described by the equation

$$\begin{aligned} -x_1 \cos \delta \sin \kappa_{\text{true}} + x_2 (\cos \gamma \cos \kappa_{\text{true}} + \sin \gamma \sin \delta \sin \kappa_{\text{true}}) \\ - x_3 (\sin \gamma \cos \kappa_{\text{true}} - \cos \gamma \sin \delta \sin \kappa_{\text{true}}) = 0, \end{aligned} \quad (25)$$

and this describes the plane of the crystal that was initially located on the reference plane. When $x_3 = 0$, thus describing the line PQ shown in Figs. 5 and 6,

$$x_2 (\cos \gamma \cos \kappa_{\text{true}} + \sin \gamma \sin \delta \sin \kappa_{\text{true}}) = x_1 \cos \delta \sin \kappa_{\text{true}}. \quad (26)$$

Thus the equation determining the intersection of the plane containing the unit vectors $\mathbf{i}_1'''$ and $\mathbf{i}_3'''$ with the $x_1 x_2$ -plane associated with the reference coordinates is given by

$$x_2 = x_1 \tan \alpha \quad \text{where} \quad \tan \alpha = \frac{\cos \delta \sin \kappa_{\text{true}}}{\cos \gamma \cos \kappa_{\text{true}} + \sin \gamma \sin \delta \sin \kappa_{\text{true}}}. \quad (27)$$

Inverting this relation leads to the following expression given in [2] determining the value of κ_{true}

$$\tan \kappa_{\text{true}} = \frac{\tan \alpha \cos \gamma}{\cos \delta - \tan \alpha \sin \gamma \sin \delta}. \quad (28)$$

The angle α can thus be measured from Laue patterns (see Fig. 5) and the corresponding value of κ_{true} can then be calculated using (28).

5. OTHER CALCULATED ANGLES

While the three angles γ , δ , and κ_{true} are sufficient to define uniquely the orientation of a cubic crystal with respect to a set of reference axes, other measures of orientation are considered by the European Gas Turbine Industry and it is useful to consider their meaning and the quantitative derivation of the relations used for their determination. The angles γ , δ , and κ_{true} define rotations of the crystal axes about each of their axes, and therefore, the ‘motion’ of their axes relative to the ‘fixed’ reference axes. In the following analysis the hat symbol, e.g. $\hat{\phi}$, will be used to denote an angle ϕ that is derived directly from a formula using the atan function, which restricts values to the range $[-\frac{\pi}{2}, +\frac{\pi}{2}]$. This value may have to be modified in order to calculate the value of ϕ that has physical significance.

European Gas Turbine Industry makes use of an angle $\hat{\omega}$ that is based on the following formula [2]

$$\tan \hat{\omega} = \frac{\sin \gamma}{\tan \delta} . \quad (29)$$

The angle $\hat{\omega}$ derived from (29) describes the direction, in the plane normal to the reference direction, of the projection parallel to the reference direction, of the unit vector $\mathbf{i}_3''$, which is the direction of the [001] crystal axis following the rotations γ and δ . It follows from (11) that the direction of this projection is defined by the vector

$$(\sin \delta, \sin \gamma \cos \delta, 0) , \quad (30)$$

that is parallel to a *unit* vector having the form

$$(\cos \hat{\omega}, \sin \hat{\omega}, 0) , \quad (31)$$

where the value of $\hat{\omega}$ must satisfy (29) and requires using the arctan function, which usually returns values lying in the range $-\frac{1}{2}\pi < \hat{\omega} < \frac{1}{2}\pi$, i.e. $(-90^\circ < \hat{\omega} < 90^\circ)$. It should be noted that when $\hat{\omega} = 0$ the unit vector defined by (31) is given by $(1, 0, 0)$, and that $\hat{\omega}$ is measured anti-clockwise when looking from the origin O towards positive values of z , as shown in Fig. 7.

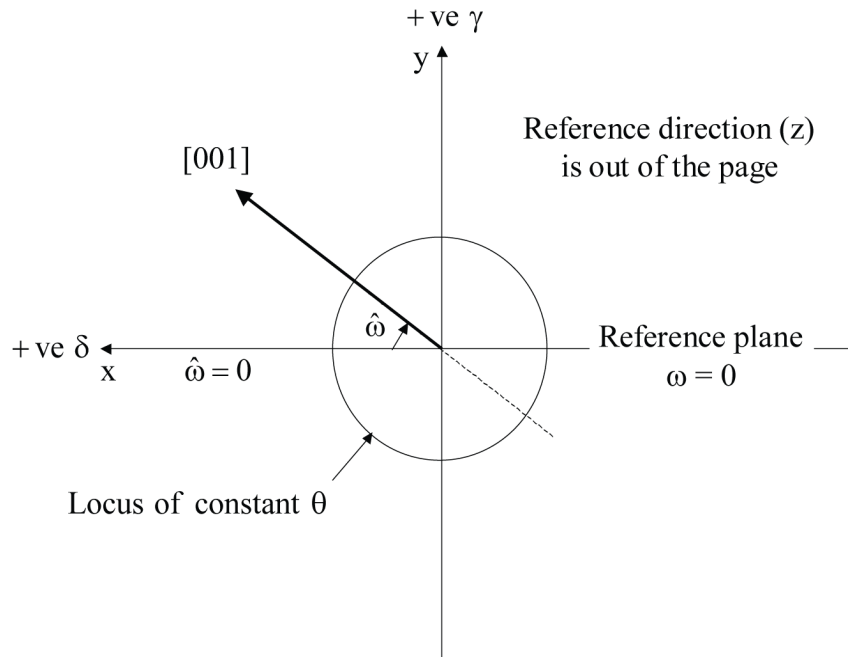


Figure 7: Diagram illustrating the meaning of the angle $\hat{\omega}$, shown for the case $\gamma > 0, \delta > 0$.

When $\hat{\omega} \rightarrow \pm\pi$, the unit vector given by (31) is in the direction of the negative values of the x-axis of the reference coordinates. The European Gas Turbine Industry uses this direction, to be the zero of an alternative angle ω , measured in the same direction as $\hat{\omega}$, that is defined for the range $0 < \omega < 2\pi$, i.e. $(0^\circ \rightarrow 360^\circ)$. Thus, ω is measured from the negative x-axis of the reference plane in a direction that is anticlockwise when looking in the reference direction from the origin towards the positive values of z . The value of ω is calculated from $\hat{\omega}$ using the relation

$$\omega = \hat{\omega} + \pi. \quad (32)$$

Consider now the angle θ that is the angle between the reference direction $\mathbf{i}_3$ and the unit vector that describes the direction of the nearest of the three principal crystal directions [100], [010], and [001] described respectively by the unit vectors $\mathbf{i}_1''', \mathbf{i}_2'''$ and $\mathbf{i}_3'''$, following the three rotational transformations. Let ϕ_1, ϕ_2 and ϕ_3 be the angles between the direction $\mathbf{i}_3$ of the original z-axis and the unit vectors $\mathbf{i}_1''', \mathbf{i}_2'''$ and $\mathbf{i}_3'''$ so that

$$\begin{aligned} \cos \phi_1 &= \mathbf{i}_1''' \cdot \mathbf{i}_3 = -\sin \gamma \sin \kappa - \cos \gamma \sin \delta \cos \kappa, \\ \cos \phi_2 &= \mathbf{i}_2''' \cdot \mathbf{i}_3 = -\sin \gamma \cos \kappa + \cos \gamma \sin \delta \sin \kappa, \\ \cos \phi_3 &= \mathbf{i}_3''' \cdot \mathbf{i}_3 = \cos \gamma \cos \delta. \end{aligned} \quad (33)$$

It should be noted that

$$\cos^2 \phi_1 + \cos^2 \phi_2 + \cos^2 \phi_3 = 1. \quad (34)$$

When determining numerically the actual values in radians of the angles ϕ_1, ϕ_2 and ϕ_3 use is made of the method specified by the relations

$$\cos \phi = u, \quad \tan \phi = \frac{\sqrt{1-u^2}}{u}, \quad \phi = \tan^{-1} \left(\frac{\sqrt{1-u^2}}{u} \right), \quad (35)$$

remembering that the symbol $\sqrt{}$ denotes the positive square root. The advantage of this method is that a unique value of ϕ is found in the range $-\pi/2 < \phi \leq \pi/2$ from the arctan function, and that negative values of ϕ will result only if $u < 0$. The relation (35) is used to determine the minimum absolute value of the angles ϕ_1, ϕ_2 and ϕ_3 , which is denoted by $\phi_{\min} \equiv \theta$. The minimum angle θ is the angle between the unit vectors $\mathbf{i}_3 = (0, 0, 1)$ and $\mathbf{i}_{\min}''' = (i_1^{\min}, i_2^{\min}, i_3^{\min})$. For practical applications it is often the case that $\phi_{\min} \equiv \theta = \phi_3$ so that from (33)

$$\cos \theta = \cos \gamma \cos \delta, \quad (36)$$

as stated in [2]. The angle θ is illustrated in Fig. 8 where the reference direction is shown relative to the crystal axes [100], [010] and [001], and the locus of constant θ is shown in Fig. 7. It can be shown that the angle θ corresponds to the angle of reflection σ shown in Fig. 1.

Some of the angles defining crystal orientation for the system used by the European Gas Turbine Industry [2] are best defined by referring them to the crystal axes as shown in Fig. 8.

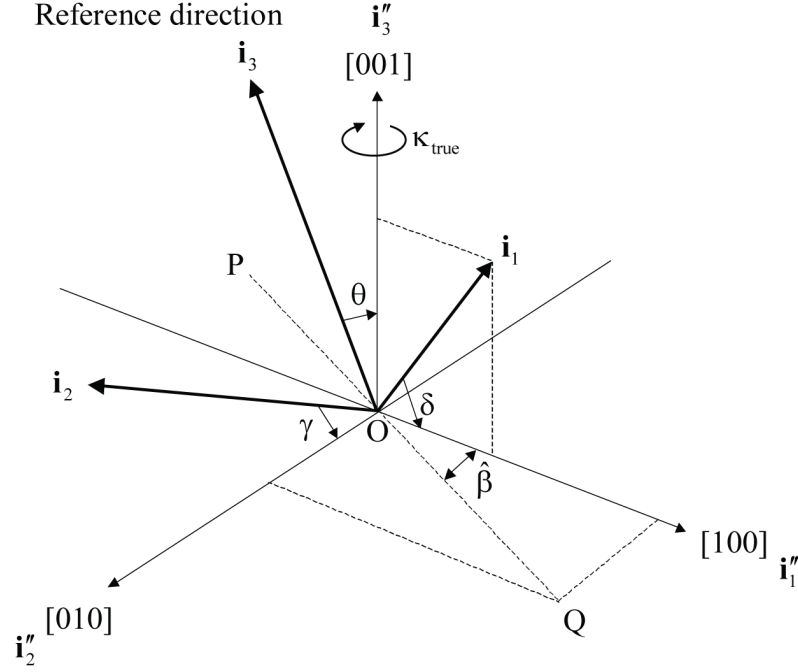


Figure 8: Diagram illustrating the angles γ , δ , θ and $\hat{\beta}$ defining crystal orientation relative to left-handed crystal axes before the κ_{true} rotation about the $[001]$ direction. The diagram is based on the intersection of the reference plane with a crystal plane and positive values of γ and δ .

The unit vectors $\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$ for the directions of the reference axes are shown in Fig. 8 together with the line PQ that is the intersection of the plane containing the unit vectors $\mathbf{i}_1$ and $\mathbf{i}_3$ (i.e. the reference plane) with the crystal plane containing the unit vectors $\mathbf{i}_1''$ and $\mathbf{i}_2''$.

From (5) and (9) it can be shown that

$$\begin{aligned} x_1 &= x_1'' \cos \delta + x_3'' \sin \delta, \\ x_2 &= -x_1'' \sin \gamma \sin \delta + x_2'' \cos \gamma + x_3'' \sin \gamma \cos \delta, \\ x_3 &= -x_1'' \cos \gamma \sin \delta - x_2'' \sin \gamma + x_3'' \cos \gamma \cos \delta. \end{aligned} \quad (37)$$

The reference plane containing the unit vectors $\mathbf{i}_1$ and $\mathbf{i}_3$ is described by the equation

$$x_2 = -x_1'' \sin \gamma \sin \delta + x_2'' \cos \gamma + x_3'' \sin \gamma \cos \delta = 0, \quad (38)$$

and its intersection with the crystal plane containing the unit vectors $\mathbf{i}_1''$ and $\mathbf{i}_2''$ is obtained by setting $x_3''=0$ in (38) so that the line PQ in Fig. 8 is described by the equation

$$-x_1'' \sin \gamma \sin \delta + x_2'' \cos \gamma = 0. \quad (39)$$

This relation is now written in the form

$$x_2'' = x_1'' \tan \gamma \sin \delta = x_1'' \tan \hat{\beta}. \quad (40)$$

As shown in Fig. 8, $\hat{\beta}$ is the angle between the line OQ and the x_1'' -axis. The crystal axes are now rotated by an angle κ_{true} in the direction shown in Fig. 8. The zero position for κ_{true} is taken as the x_1'' -axis. The x_1'' -axis will, therefore, rotate so that it makes an angle κ_{true} with the position of the x_1'' -axis after just the γ and δ rotations. An angle κ is used by the European Gas Turbine Industry [2] that is the κ_{true} rotation measured relative to the position OQ of the reference plane after just the γ and δ rotations. It then follows, on using (40), that

$$\kappa = \kappa_{\text{true}} - \hat{\beta}, \quad \text{where} \quad \tan \hat{\beta} = \tan \gamma \sin \delta, \quad (41)$$

as defined in reference [2].

An additional angle used by the European Gas Turbine Industry will now be defined by projecting the reference direction onto the plane containing the two unit vectors describing the transformed crystal directions that are normal to the [001] direction following the γ and δ rotations, but before the final κ_{true} rotation occurs (see Fig. 9). It is emphasised that the unit vectors $\mathbf{i}_3, \mathbf{i}_3''$ and the line OP shown in Fig. 9 are coplanar. The relations (12) are now considered, namely,

$$\begin{aligned} \mathbf{i}_1 &= \cos \delta \mathbf{i}_1'' + \sin \delta \mathbf{i}_3'', \\ \mathbf{i}_2 &= -\sin \gamma \sin \delta \mathbf{i}_1'' + \cos \gamma \mathbf{i}_2'' + \sin \gamma \cos \delta \mathbf{i}_3'', \\ \mathbf{i}_3 &= -\cos \gamma \sin \delta \mathbf{i}_1'' - \sin \gamma \mathbf{i}_2'' + \cos \gamma \cos \delta \mathbf{i}_3'', \end{aligned} \quad (42)$$

which show how the unit vectors of the reference axes may be obtained from those of the crystal axes following the γ and δ rotations.

The projection parallel to the $\mathbf{i}_3''$ direction of the unit vector $\mathbf{i}_3$ describing the reference direction, onto the plane containing the unit vectors $\mathbf{i}_1''$ and $\mathbf{i}_2''$ defining the crystal directions, is described by the vector

$$(-\cos \gamma \sin \delta, -\sin \gamma, 0). \quad (43)$$

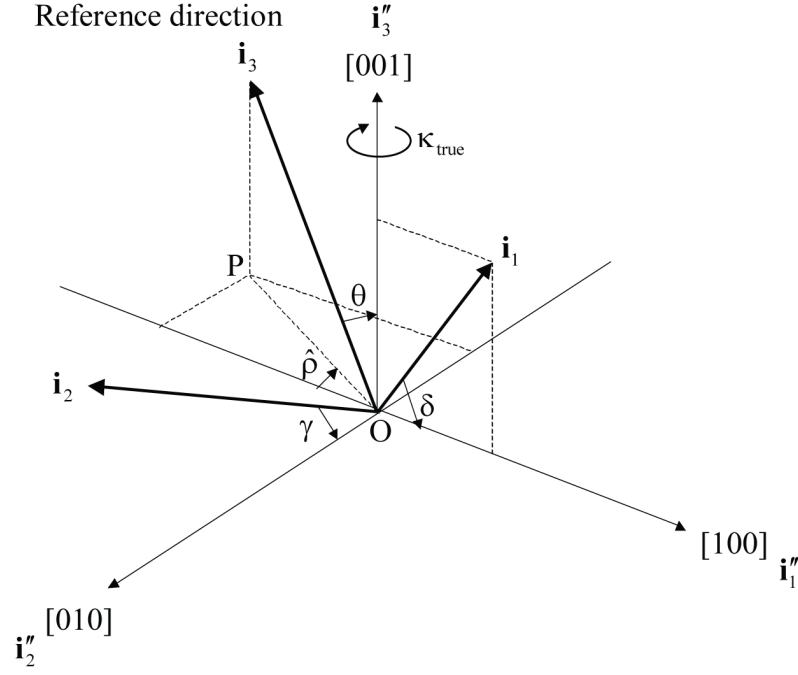


Figure 9: Diagram illustrating the angles γ , δ , θ and $\hat{\rho}$ defining crystal orientation relative to left-handed crystal axes before the κ_{true} rotation about the $[001]$ direction.

The diagram is based on projections of the unit vector $\mathbf{i}_3$ onto a crystal plane and positive values of γ and δ .

The above vector describing the projection is not a unit vector, but a corresponding *unit* vector can be defined by

$$(-\cos \hat{\rho}, -\sin \hat{\rho}, 0), \quad (44)$$

where

$$\tan \hat{\rho} = \frac{\tan \gamma}{\sin \delta}. \quad (45)$$

With respect to the crystal axes, the projection of the unit vector $\mathbf{i}_3$ for the reference direction onto the plane normal to the $[001]$ crystal direction (see Fig. 9) defines a line OP that is inclined at an angle $\hat{\rho}$ to the $[100]$ crystal direction. Using a left-hand set of crystal axes, $\hat{\rho}$ is defined to be positive when it is measured from the origin along the x_1'' -axis ($[100]$ direction) in a direction that is anti-clockwise when looking from the origin along x_3'' -axis ($[001]$ direction) as shown in Fig. 9. Following the rotation about the $[001]$ direction by an angle κ_{true} the line OP will move so that it is inclined at an angle ρ' to the negative x_2'' -axis where

$$\rho' = \hat{\rho} + \kappa_{\text{true}}. \quad (46)$$

Having found, using (45), the value of $\hat{\rho}$ with respect to the given crystal axes, the value of $\rho' = \hat{\rho} + \kappa_{\text{true}}$ is then calculated. The angle ρ' must then be adjusted by

adding or subtracting 2π , (360°), so that the adjusted value lies in the range $-\pi < \rho' \leq \pi$, i.e. ($-180^\circ < \rho' \leq 180^\circ$). The adjusted angle will define the direction of the projection of the reference direction onto the plane containing the [100] and [010] crystal directions. The required angle ρ is defined to be the angle between the direction of the projected reference direction and the *nearest* of the crystal axes [100] and [010]. The value of ρ is such that $0 \leq \rho \leq \frac{\pi}{4}$, i.e. ($0^\circ \leq \rho \leq 45^\circ$). The method for determining the appropriate value of ρ is shown in Table 1, given a value of ρ' in the range $-\pi < \rho' \leq \pi$, i.e. ($-180^\circ < \rho' \leq 180^\circ$), obtained from (46).

Table 1: Method of determining value of ρ from ρ' .

Angle range (radians/degrees)	ρ
$-\pi < \rho' \leq -\frac{3}{4}\pi$, ($-180^\circ < \rho' \leq -135^\circ$)	$\pi + \rho'$
$-\frac{3}{4}\pi < \rho' \leq -\frac{1}{2}\pi$, ($-135^\circ < \rho' \leq -90^\circ$)	$-\frac{1}{2}\pi - \rho'$
$-\frac{1}{2}\pi < \rho' \leq -\frac{1}{4}\pi$, ($-90^\circ < \rho' \leq -45^\circ$)	$\frac{1}{2}\pi + \rho'$
$-\frac{1}{4}\pi < \rho' \leq 0$, ($-45^\circ < \rho' \leq 0^\circ$)	$-\rho'$
$0 < \rho' \leq \frac{1}{4}\pi$, ($0^\circ < \rho' \leq 45^\circ$)	$+\rho'$
$\frac{1}{4}\pi < \rho' \leq \frac{1}{2}\pi$, ($45^\circ < \rho' \leq 90^\circ$)	$\frac{1}{2}\pi - \rho'$
$\frac{1}{2}\pi < \rho' \leq \frac{3}{4}\pi$, ($90^\circ < \rho' \leq 135^\circ$)	$-\frac{1}{2}\pi + \rho'$
$\frac{3}{4}\pi < \rho' \leq \pi$, ($135^\circ < \rho' \leq 180^\circ$)	$\pi - \rho'$

6. CONCLUSION

A mathematical representation, to describe rigorously the orientation angles of cubic crystals, has been developed, which can be used as the basis of defining unambiguously various angles of rotation that are employed by the European Gas Turbine Industry.

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APPENDIX 1: Description of resolution of vectors

As the various transformations given in this report have made use of the resolution of unit vectors, it is useful to describe for general readers the methodology used. Fig. A1 shows the first transformation of axes that was considered in this report.

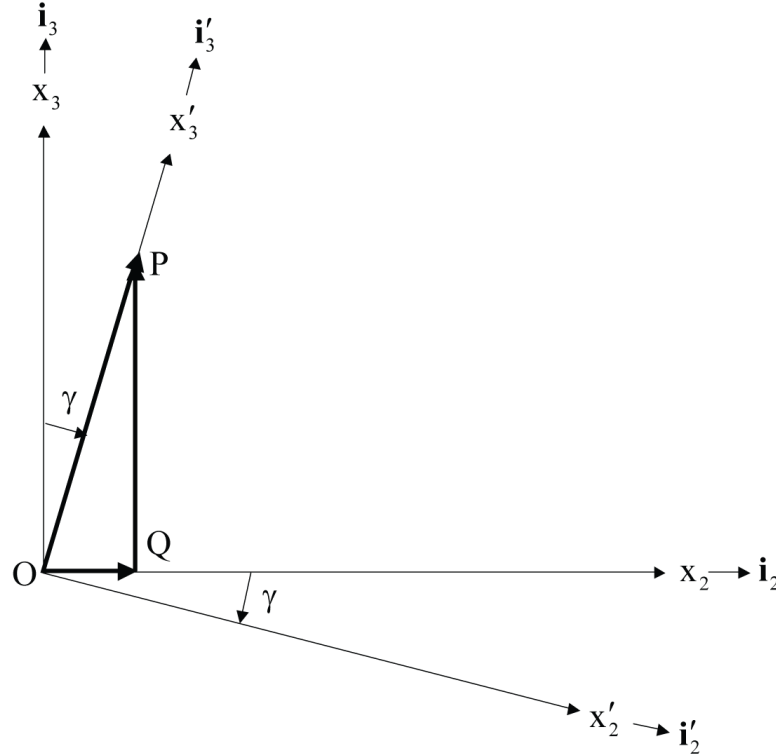


Figure A1: Diagram illustrating resolution of a unit vector into unit vectors for a different orientation of axes.

The vector $\overline{OP}$ is a unit vector for the x'_3 direction of the transformed axes. The vector $\overline{OQ}$ acts along the x_2 -axis and has magnitude OQ while the vector $\overline{QP}$ acts in the direction of the x_3 -axis and has magnitude PQ . Since γ is the angle of rotation of the axes, and since OP is of unit length, it follows that $OQ = \sin \gamma$ and $PQ = \cos \gamma$. Thus, $\overline{OQ} = \sin \gamma \mathbf{i}_2$ and $\overline{QP} = \cos \gamma \mathbf{i}_3$. The vector addition rule is written $\overline{OP} = \overline{OQ} + \overline{QP}$ leading to the relation

$$\mathbf{i}'_3 = \sin \gamma \mathbf{i}_2 + \cos \gamma \mathbf{i}_3.$$

Relations of this type are used repeatedly in this report.